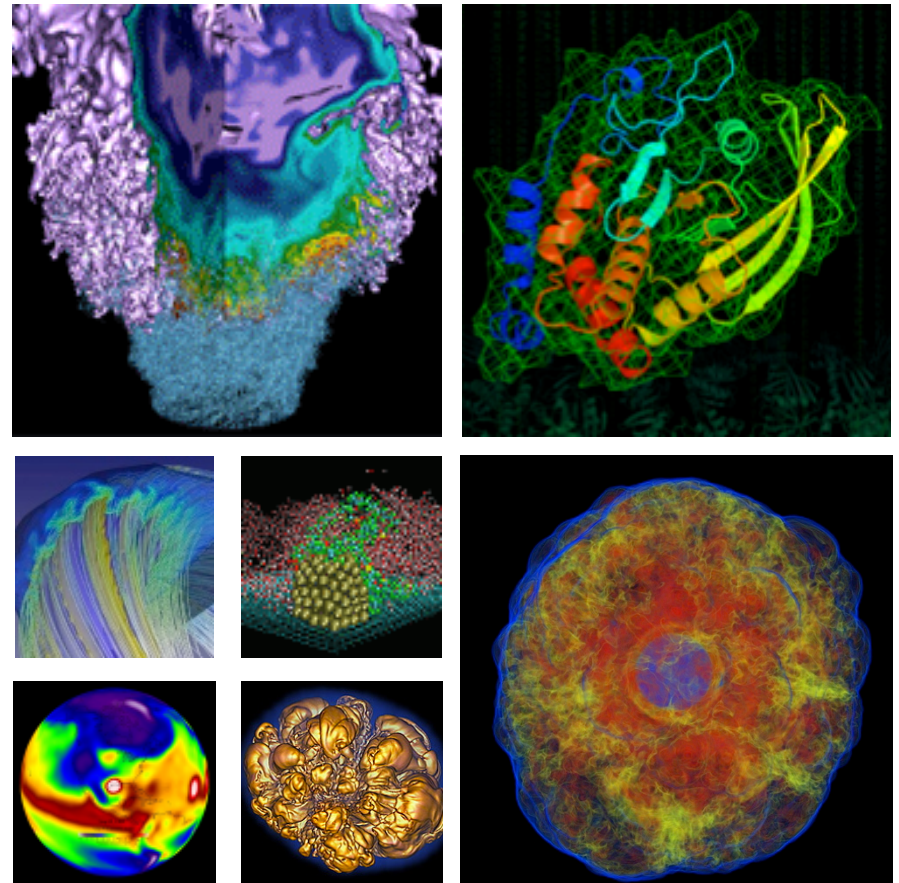
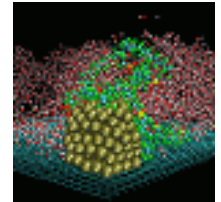
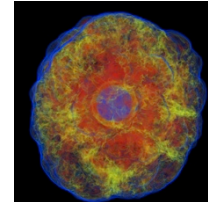
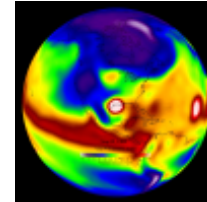
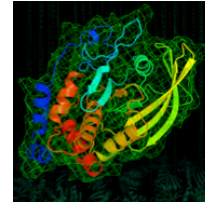
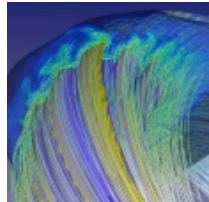
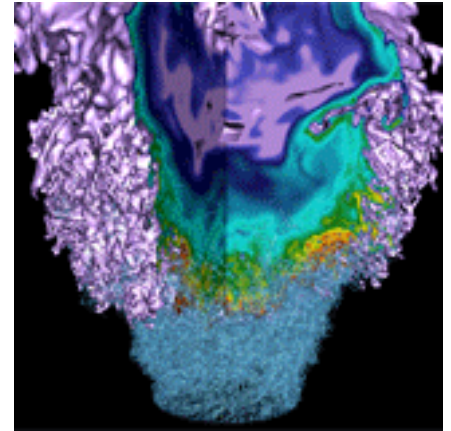


Moving And Sharing Data at NERSC



Shreyas Cholia
scholia@lbl.gov
Data and Analytics Services
New User Training 2016
March 21th, 2016

Data Transfer Nodes



Dedicated Data Transfer Systems:

Data Transfer Nodes



- **Data Transfer Nodes (DTN) are servers dedicated to data transfer at NERSC.**
 - Currently 4 Nodes → `dtn[01-04].nersc.gov`
 - **DTN features**
 - High bandwidth network interfaces
 - Access to global NERSC file systems
 - Tuned for efficient data transfers
 - Tuned for transferring large volumes of data between NERSC and other major facilities (ORNL, ANL etc.)
 - Can also move data between NERSC file systems and HPSS
- **Use the DTNs if you want to move large volumes of data in and out of NERSC**

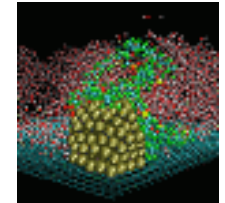
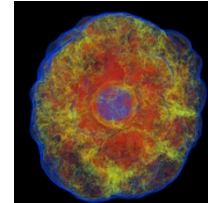
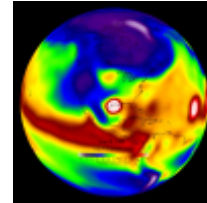
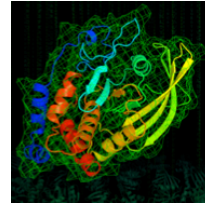
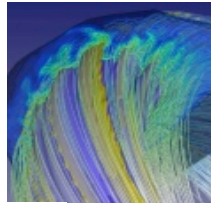
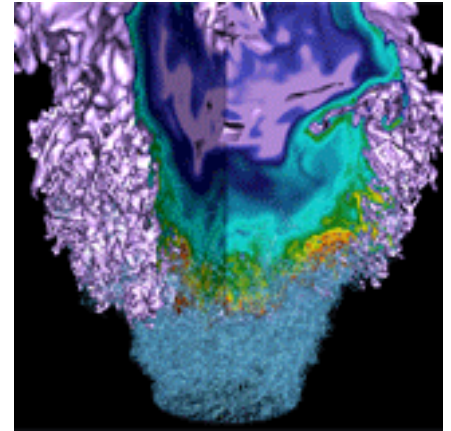
DTN Login Access



- **All NERSC users have login access**
 - NERSC Users (non-JGI):
 - `ssh dtn01.nersc.gov` (or `dtn02`)
 - JGI Users:
 - `ssh dtn03.nersc.gov` (or `dtn04`)
- **Familiar module environment**
 - `module avail`
 - Limited software deployment for data transfer needs

- **Global File Systems are available**
 - /global/homes
 - /global/project
 - /global/projecta
 - /global/projectb
 - /global/dna
 - /global/seqfs
 - /global/common
- **Currently excludes system-specific file systems**
 - e.g. /scratchX on Cori & Edison

Moving Data

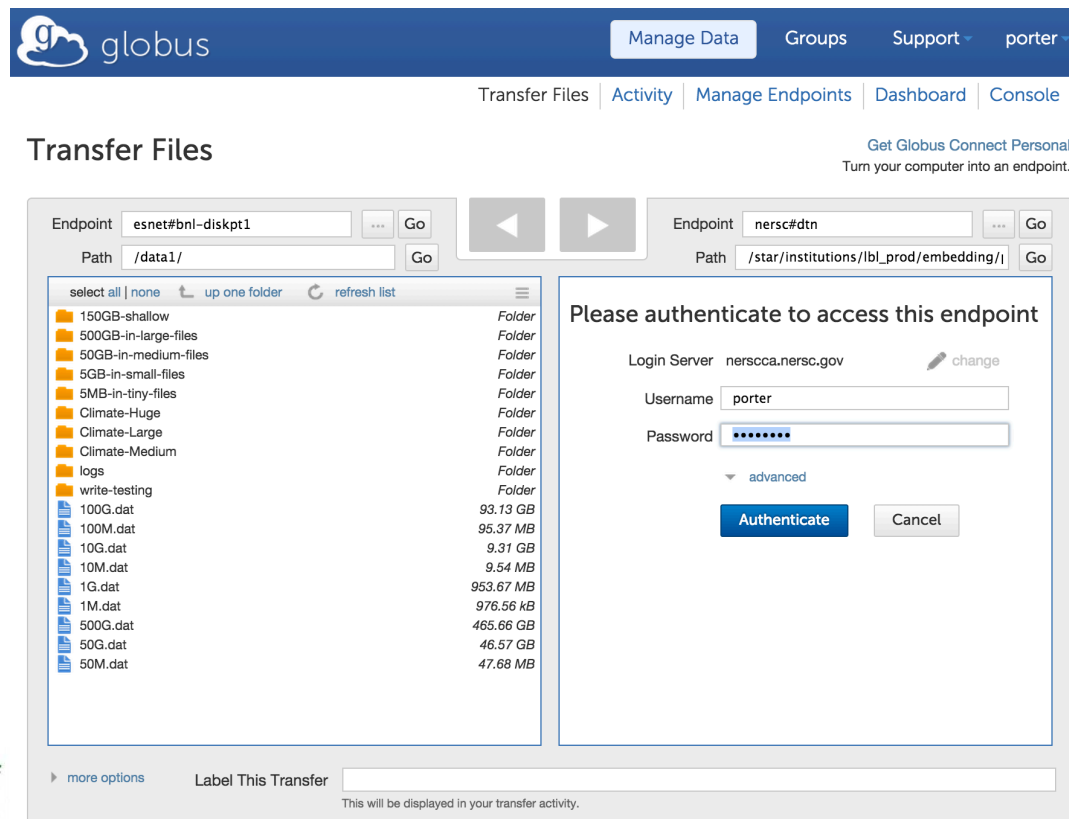


Transfer Tools

- **Globus: <http://globus.org>**
 - Reliable transfers of large data sets between sites or systems
- **scp**
 - copying individual files and directories
- **GridFTP (globus-url-copy)**
 - high performance CLI w/ grid certificates
- **bbcp**
 - high performance CLI tool w/ minimal setup
- **hsi/htar**
 - for data transfer into & out of HPSS



- **Managed 3rd party transfers** <https://www.globus.org/>
 - Web based interface, currently requires Globus Account
- **Type nersc#dtn endpoint in the transfer window**
 - Activate with NERSC username & password



The screenshot shows the Globus web interface. At the top, there's a navigation bar with the Globus logo and links for Manage Data, Groups, Support, and porter. Below this, there's a secondary navigation bar with links for Transfer Files, Activity, Manage Endpoints, Dashboard, and Console. The main content area is titled "Transfer Files" and includes a link to "Get Globus Connect Personal" with the text "Turn your computer into an endpoint."

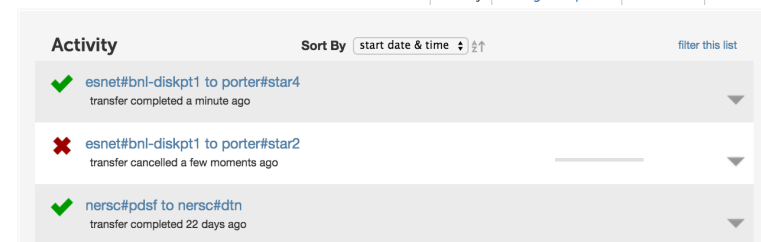
The interface is divided into two main sections. The left section shows a file browser for the endpoint "esnet#bnl-diskpt1" at the path "/data1/". It lists various folders and files, including "150GB-shallow", "500GB-in-large-files", "50GB-in-medium-files", "5GB-in-small-files", "5MB-in-tiny-files", "Climate-Huge", "Climate-Large", "Climate-Medium", "logs", "write-testing", and several ".dat" files of varying sizes.

The right section shows a file browser for the endpoint "nersc#dtn" at the path "/star/institutions/lbl_prod/embedding/". It displays an authentication dialog titled "Please authenticate to access this endpoint". The dialog includes fields for "Login Server" (nerscca.nersc.gov), "Username" (porter), and "Password" (masked with dots). There are "Authenticate" and "Cancel" buttons, and a link for "advanced" options.

At the bottom of the interface, there's a "Label This Transfer" field and a note: "This will be displayed in your transfer activity."

Globus.org Continued

- **Use point & click interface to submit**
 - Transfer happens in the background & retries on failure
 - You can status on Activity panel
 - Email notification on completion



Globus Notification

To: Jeff Porter

SUCCEEDED - 20d4f522-41e3-11e5-acba-22000b92c6ec

TASK DETAILS

Task ID : 20d4f522-41e3-11e5-acba-22000b92c6ec
 Task Type : TRANSFER
 Status : SUCCEEDED
 Is Paused : No
 Request Time : 2015-08-13 17:45:47Z
 Deadline : 2015-08-14 17:45:46Z
 Completion Time : 2015-08-13 17:46:08Z
 Total Tasks : 1
 Tasks Successful : 1
 Tasks Expired : 0
 Tasks Canceled : 0
 Tasks Failed : 0
 Tasks Pending : 0
 Tasks Retrying : 0
 Command : API 0.10 go
 Label : n/a
 Source Endpoint : esnet#bnl-diskpt1
 Destination Endpoint : porter#star4
 Sync Level : n/a
 Data Encryption : No
 Checksum Verification : Yes
 Delete : No
 Files : 1
 Files Skipped : 0
 Directories : 0
 Expansions : 0
 Bytes Transferred : 1000000000
 Bytes Checksummed (Sync): 0
 Effective MBits/sec : 380.952
 Faults : 0

- **Globus Connect allows a private endpoint on your laptop**
 - <https://www.globus.org/globus-connect>

Other tools

- **Command line tools for use directly from the DTN nodes or from a remote node**
 - scp
 - <http://tinyurl.com/nersc-gridftp>
 - GridFTP (globus-url-copy)
 - <http://tinyurl.com/nerscbbcp>
- **Detailed instructions, syntax etc.**
 - <http://tinyurl.com/nerscdtn>

Tool	Throughput
scp	140 Mbps (17.5 MB/s)
HPN patched scp , 1 disk	760 Mbps (95 MB/s)
HPN patched scp , RAID disk	1.2 Gbps (150 MB/s)
GridFTP, 1 stream, 1 disk	760 Mbps (95 MB/s)
GridFTP, 1 stream, RAID disk	1.4 Gbps (175 MB/s)
GridFTP, 4 streams, RAID disk	5.4 Gbps (675 MB/s)
GridFTP, 8 streams, RAID disk	6.6 Gbps (825 MB/s)

<http://fasterdata.es.net/data-transfer-tools/>

scp - Secure Copy

- Uses SSH under the covers
- Good for “small” (~100s of MB)
- Simple cp-like syntax
 - `scp localfile user@host:remotefile`
- At NERSC, we deploy high performance modifications (HPN SSH) to get better throughput

- **Backup or archive your data with HSI and HTAR**
<http://www.nersc.gov/users/data-and-file-systems/hpss/getting-started/>
(<http://tinyurl.com/nerschpss>)
- **Login to DTN node and use hsi/htar**
 - HSI for individual files and conditional access
 - HTAR for aggregation & optimization of storage/archival
- **Can also use Globus Online:**
 - External endpoint \leftrightarrow nersc#hpss
 - nersc#dtn \leftrightarrow nersc#hpss
 - But individual files only, does not support htar

General Tips

- **Use DTNs as dedicated data transfer servers**
 - Tuned for WAN transfers
 - Fast network (ESnet), optimized configuration
 - See <http://fasterdata.es.net/> for more discussion
 - Dedicated support for data transfer
- **Don't use DTN nodes for non-data transfer purposes**
- **Use Globus for large, automated or monitored transfers**
- **scp is fine for smaller, one-time transfers (<100MB)**
 - Globus is also fine for small transfers
- **Plain “cp” or “rsync” is still used for local transfers**

Performance Considerations

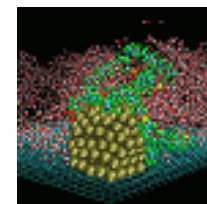
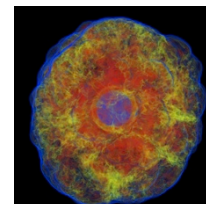
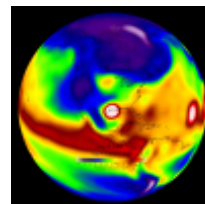
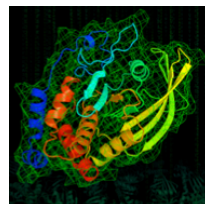
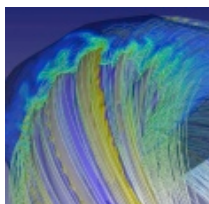
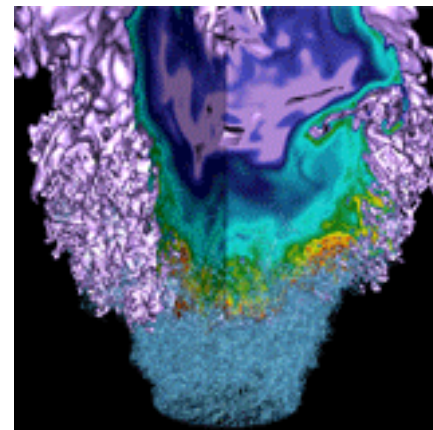


- **Performance is often limited by the remote endpoint**
 - Not tuned for WAN transfers
 - Have limited network (~1Gb/sec) link.
 - These will lower performance < 100 MB/sec.
- **File system contention may be an issue**
 - For example, don't use your \$HOME directory!
 - Instead use /project, \$SCRATCH or \$GSCRATCH
- **If you don't think you are getting the performance you expect, let us know: consult@nersc.gov**

For more information

- **General DTN info**
 - <http://www.nersc.gov/systems/data-transfer-nodes/>
- **Data transfer info**
 - <http://www.nersc.gov/users/data-and-file-systems/transferring-data/>
(or <http://tinyurl.com/nerscdtn>)
- **Feedback / Problems?**
 - consult@nersc.gov
- **Globus Support**
 - <https://www.globus.org/support/>

Uploads from Outside Users

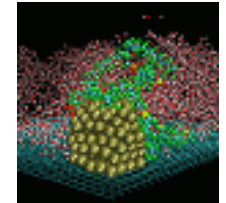
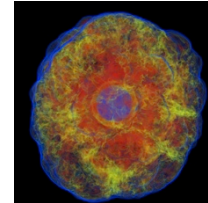
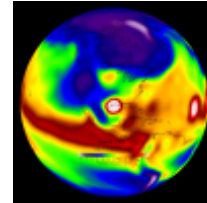
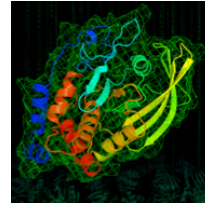
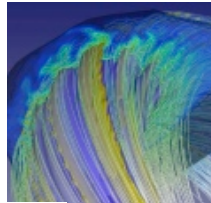
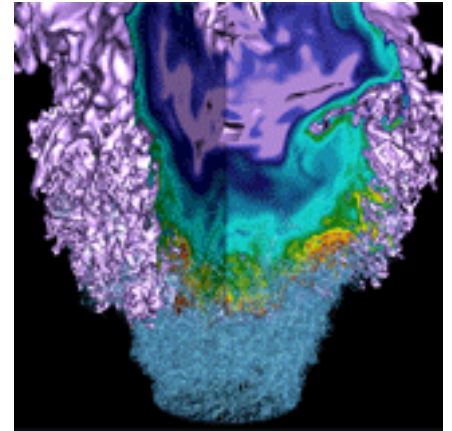


Anonymous FTP Upload Service



- For external collaborators to be able to send data to NERSC users
- Create a temporary FTP account to upload files that will be delivered to a NERSC user
- NERSC user can retrieve the file:
`take -u ftpup <file_name>`
- <https://www.nersc.gov/users/storage-and-file-systems/transferring-data/nersc-ftp-upload-service>

Sharing Data Within NERSC



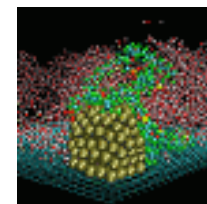
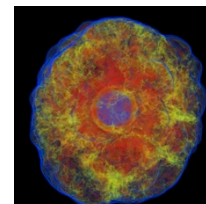
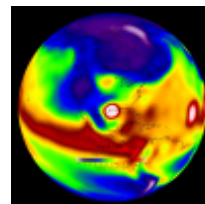
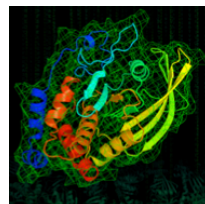
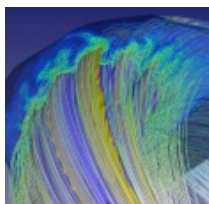
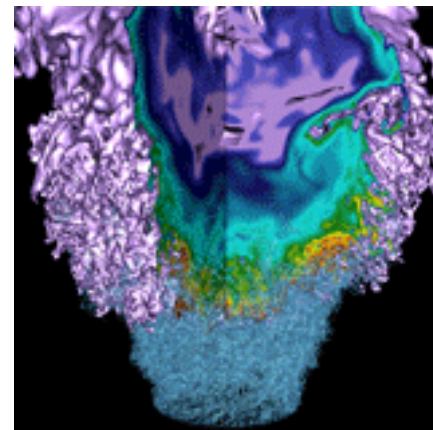
The /project directory



- Your project will have a shared project directory at `/global/project/projectdirs/<dirname>`
- Shared group permissions for your project repo
- <https://www.nersc.gov/users/storage-and-file-systems/sharing-data/>

- **Give a file to a user:**
 - give -u <recipient-username> <file-or-directory>
 - This sends is into a holding area for pickup and notifies the recipient over email
- **Accept a file from a user**
 - take -u <sender-username> (-d <destination folder>) <filename>
 - Picks up the file (use -a for all files)


Science Gateways: Sharing Data over the Web














NERSC Science Gateways



- Web portals that allow you to interface with your data and computation at NERSC
- Interfaces built around your science
- Science-As-A-Service

 **Science Gateways**

NERSC science gateways bring the work of our users to collaborators and the world. Many are open access; others require a login. Explore the gateways themselves for more about each project and how to access data.

	The Materials Project cite		20th Century Reanalysis cite
	DeepSky		Dayabay
	QCD		Earth System Grid cite
	CXIDB		OpenMSI
	NOVA		NEWT
	ALS Spot Portal		

- Simple data publishing capabilities
- Rich web interfaces and complex portals
- Backend databases and message queues
- **Interactive Analysis Tools over the Web**
 - iPython Notebooks and R Studio
- **NEWT API to access NERSC resources**

Publish Data On the Web

- Every repo now has a project directory
- Trivial to wire up your project directory to make it accessible over the web
- Create a file in your www directory
 - mkdir /global/project/projectdirs/<yourproj>/www
 - cd /global/project/projectdirs/<yourproj>/www
 - vi index.html
 - <html>Hello World</html>
- Make sure all the above files and directories are world readable
 - chmod 775 /global/project/projectdir/<yourproj>/ etc.
- Voila:
 - <http://portal.nersc.gov/project/<yourproj>/>

Build Full Stack Web Applications



- **Build full stack web applications for your science at NERSC**
 - **Python/Django, PHP**, Ruby on Rails, Java Backends
 - JavaScript + AJAX Frontends
- **Databases**
 - MongoDB, MySQL, PostGreSQL, SciDB
 - <http://tinyurl.com/nerscdbs>
- **Public or Authenticated Gateways**
 - <http://portal.nersc.gov> OR <https://portal-auth.nersc.gov>
- **OpenDAP and MQ services**

Use NEWT API to access NERSC

- NEWT – the NERSC REST API
- Use the NEWT HTTP API to access NERSC HPC resources directly from your web apps.

Example:

GET <https://newt.nersc.gov/newt/status/>

```
[{"status": "up", "system": "cori" },  
 { "status": "up", "system": "edison" },  
 { "status": "up", "system": "pdsf" },  
 { "status": "up", "system": "genepool" },  
 { "status": "up", "system": "archive"}]
```

NEWT Features

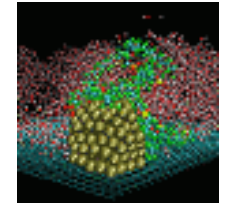
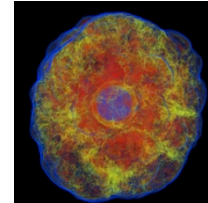
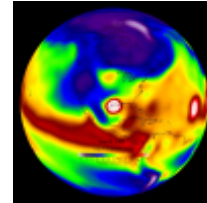
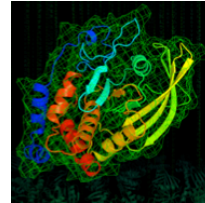
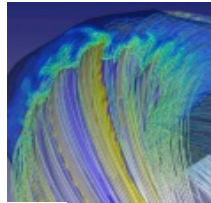
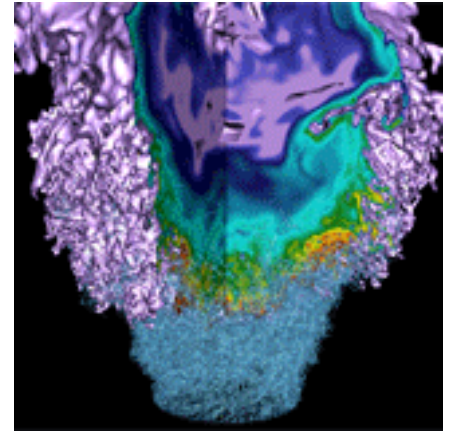
- **Run Commands on any system**
- **Transfer files**
- **Authentication**
- **Submit/Query Jobs directly through NEWT**
- **Persistent Store**
 - Store JSON objects in the NEWT storage
- **Access to NIM info**
 - Information about Users, Repos etc.
- **System Status**



Some Examples

- <http://materialsproject.org>
- <https://spot.nersc.gov>
- <https://openmsi.nersc.gov>
- <https://newt.nersc.gov/> for NEWT documentation and live demos

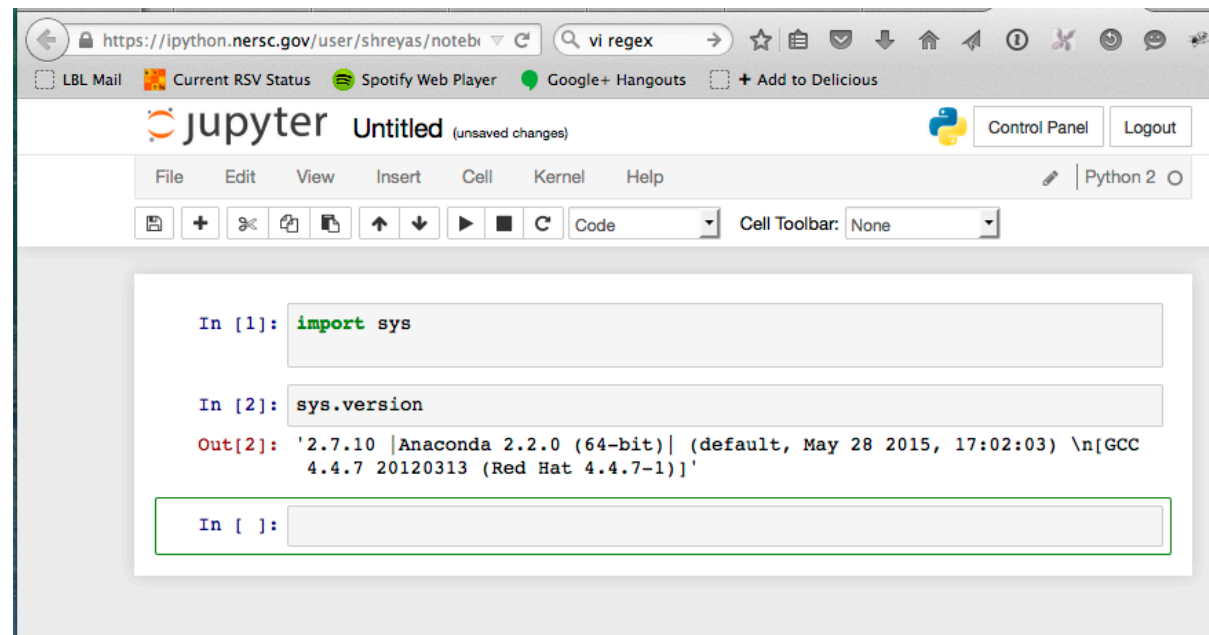
Interactive Environments



Jupyterhub – iPython Notebook Service



- Jupyter server with access to NERSC resources
 - <https://ipython.nersc.gov>
 - Login with NERSC credentials
- Access to NERSC global filesystems
- Runs inside NERSC network



- <https://r.nersc.gov>

The screenshot displays the R Studio web interface. The top menu bar includes File, Edit, Code, View, Plots, Session, Build, Debug, Tools, and Help. The user is logged in as 'shreyas' and the project is '(None)'. The console shows the following R code and output:

```
[1] "character"
> 1i
[1] 0+1i
> 1:10
[1] 1 2 3 4 5 6 7 8 9 10
> a <- 1:10
> a
[1] 1 2 3 4 5 6 7 8 9 10
> a <- a + 1
> a
[1] 2 3 4 5 6 7 8 9 10 11
> b <- a + 1
> b
[1] 3 4 5 6 7 8 9 10 11 12
> a
[1] 2 3 4 5 6 7 8 9 10 11
> a + b
[1] 5 7 9 11 13 15 17 19 21 23
> c = c(0.1, 0.2)
> a + c
Error in a + c : non-numeric argument to binary operator
> a + c
[1] 2.1 3.2 4.1 5.2 6.1 7.2 8.1 9.2 10.1 11.2
> c + a
[1] 2.1 3.2 4.1 5.2 6.1 7.2 8.1 9.2 10.1 11.2
> a - mean(a)
[1] -4.5 -3.5 -2.5 -1.5 -0.5 0.5 1.5 2.5 3.5 4.5
> rep(3, 5)
[1] 3 3 3 3 3
> rep(1, 20)
[1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
> c(rep(1,20), a)
[1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 3 4 5 6 7 8 9 10 11
19 Dec 2015 03:36:36 [rsession-shreyas] ERROR session hadabend; LOGGED FROM: core::Error<unnamed>::
rInit(const r::session::RInitInfo&) /root/rstudio/src/cpp/session/SessionMain.cpp:1694
> |
```

The Environment pane on the right shows the following variables:

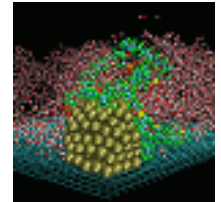
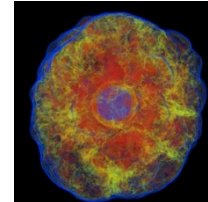
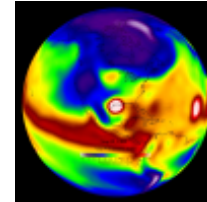
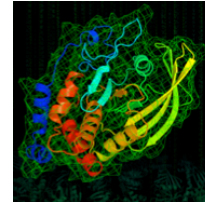
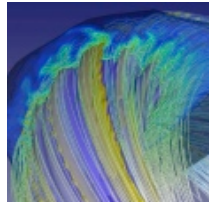
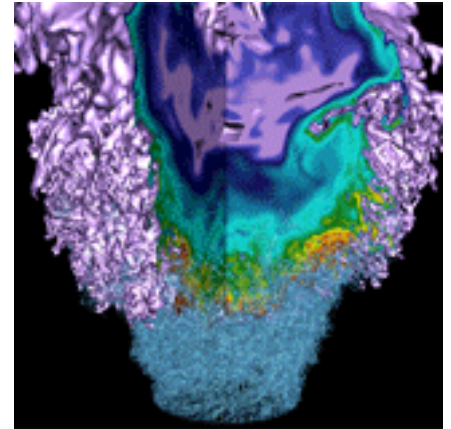
Variable	Class	Value
a	num [1:10]	2 3 4 5 6 7 8 9 10 11
b	num [1:10]	3 4 5 6 7 8 9 10 11 12
c	num [1:2]	0.1 0.2
s	"w"	

The Files pane on the right shows a list of files and folders in the current directory:

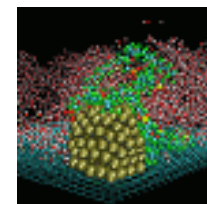
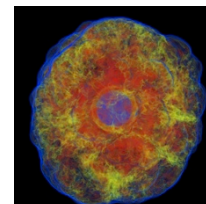
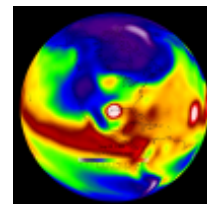
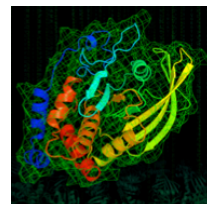
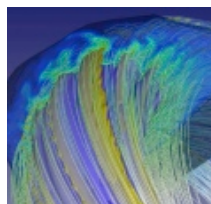
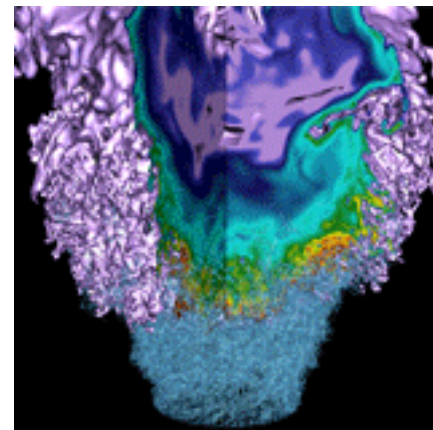
Name	Size	Modified
.Rhistory	25 B	Jul 16, 2013, 1:24 PM
.Rprofile	232 B	Jul 16, 2013, 1:15 PM
10637574.cvrsvc09-ib.ER	0 B	Nov 13, 2014, 9:01 AM
10637574.cvrsvc09-ib.OU	701 B	Nov 13, 2014, 9:01 AM
10637809.cvrsvc09-ib.ER	0 B	Nov 13, 2014, 9:19 AM
10637809.cvrsvc09-ib.OU	704 B	Nov 13, 2014, 9:19 AM
10638128.cvrsvc09-ib.ER	0 B	Nov 13, 2014, 10:09 AM
10638128.cvrsvc09-ib.OU	704 B	Nov 13, 2014, 10:10 AM
10638214.cvrsvc09-ib.ER	0 B	Nov 13, 2014, 10:34 AM
10638214.cvrsvc09-ib.OU	704 B	Nov 13, 2014, 10:34 AM
1M.dat	976.6 KB	Sep 16, 2015, 11:50 AM
2.7.3	1.6 KB	Mar 19, 2015, 10:51 AM
20C		
51_ftp-gsi		
access.wsgi	1.6 KB	Jun 28, 2011, 1:18 PM

- **There are various levels of engagement and collaboration**
 - Level 1: NERSC provides building blocks and backend infrastructure, science groups build their own gateways.
 - Level 2: NERSC offers some initial consulting help to get you started.
 - Level 3: Immersive development - science groups work in collaboration with NERSC engineers to build gateways. (But requires more resources from both sides).
- **If you are interested in building a portal please come and talk to us. We can help customize our offerings to meet user needs.**
 - Customized VMs, URLs, Docker deployments

Thanks



Extra



- **Grid tools available on NERSC systems via “module load globus”**
 - globus-url-copy
 - <http://tinyurl.com/nersc-gridftp>
- **Use Data Transfer nodes for wide-area transfers**
 - dtn01.nersc.gov
 - dtn02.nersc.gov
 - dtn03.nersc.gov
 - dtn04.nersc.gov
- **Use “grid” name for system specific file systems (often not optimal solution)**
 - corigrid.nersc.gov
 - edisongrid.nersc.gov
 - pdsfgrid.nersc.gov

BaBar Copy (bbcp)



- **Developed for BaBar experiment at SLAC**
 - Somewhat complicated command-line
 - <https://www.nersc.gov/users/data-and-file-systems/transferring-data/bbcp/>
 - <http://tinyurl.com/nerscbbcp>
- **Peer-to-peer model (not client-server)**
 - Must be installed on each end
 - Easy to build and/or install
 - Available on all NERSC systems
 - Can do third-party transfers
 - Uses ssh authentication
 - Good for larger files